

**Physics**  
**THEORETICAL NEUROSCIENCE: MODELING THE ACTIVATION**  
**MECHANISM OF POTASSIUM CHANNELS IN NEURONS**

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We have modeled the electrostatic interaction between the S4 segment of the potassium channel molecule and the surrounding water molecules on both the intracellular and extracellular sides of the neural axon cell membrane. Two methods were used to approximate this interaction: (i) a macroscopic evaluation in which the water was treated as a dielectric medium with dielectric constant 80; (ii) a microscopic evaluation considering the effects of each individual water molecule fixed in position within the water pockets surrounding the S4 segment. The potential energy of the S4 due to the water pockets was plotted against the rotation of the S4 segment, while keeping the water pockets in their fixed positions. Although the two methods gave some differing results, both methods produced single well potential energy curves of  $\sim 4$ -8 eV depth. Based on this energy curve, we show that other forces on the S4 must create an effective torsional spring force with spring constant  $k \sim 2$ -4 eV in order to produce a two well potential energy curve in qualitative agreement with experimental data.